

The Evolution of the ESRF's Structural Biology Beamlines.

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Overview

1 ESRF Upgrade

2 Structural Biology in the Upgrade.

3 Evolution

without whom

- Gordon Leonard
- ID14-1 - Xavier Thibault
- ID14-2 - Matthew Bowler
- ID14-3 - Petra Pernot / Adam Round (EMBL)
- ID14-4 - Andrew McCarthy (EMBL) / Sandor Brockhauser (EMBL)
- ID23-1 - Sasha Popov / Daniele de Sanctis
- ID23-2 - David Flot
- ID29 - Christoph Mller-Dieckmann / Daniele de Sanctis
- Joanna Timmins
- Didier Nurizzo
- David Flot
- Joanna Timmins
- Debby Davison
- Claudine Romero
- Laurence Serre
- Trevor Mairs
- Pascal Thevenneau
- Werner Schmid
- John Surr
- Thierry Giraud
- Fabien Dobias
- Mario Lentini
- Antonia Beteva
- Ricardo Nogueira Fernandes
- Darren Spruce
- Matias Guijarro
- Ulrike Kapp
- Samira Acajaoui
- Elspeth Gordon
- Stephanie Malbet-Monaco
- Gianluca Cioci
- Ed Mitchell
- Mats Ökvist (NORSTRUCT)
- Antoine Royant (IBS Cryobench)
- Martin Weik (Cryobench)
- Kjersti Lien (NORSTRUCT)
- Carlo Petosa (IBS)
- Douglas Juers (IBS/Whitman College)
- Cyril Dian (IBS)
- Anna-Maria Goncalves
- Jens Radzimanowski
- Meike Stelter
- Tobias Klar
- Ricardo Leal
- Dario Piano
- Sofia Caria
- Amandine Lallemand
- Tommaso Tosi
- Simone Pellegrino
- Rita Giordano
- Joana Rocha
- Deeksha Munnur
- Isabel Baker

ESRF Upgrade 2009 – 2015

- Major Scientific Themes.
- Machine Developments.
- New Instruments matching Scientific Priorities.
- Partnerships and Supporting Facilities.
- Further regeneration of the International site.

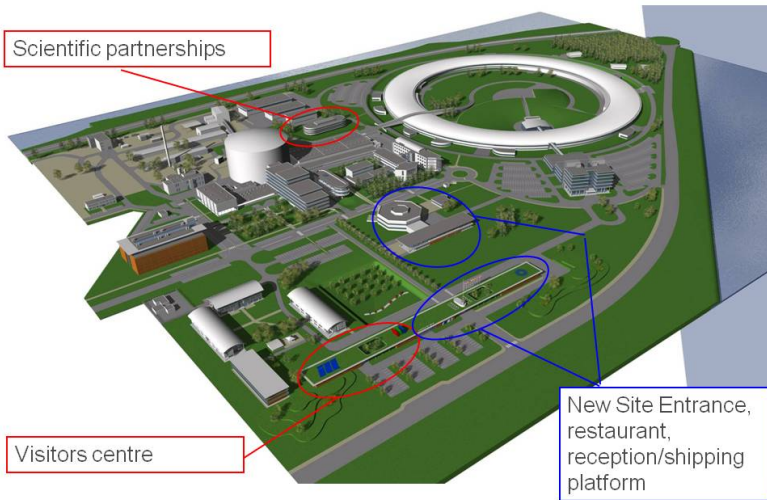
More Info?

<http://www.esrf.eu/Upgrade>

Scientific Priority Themes.

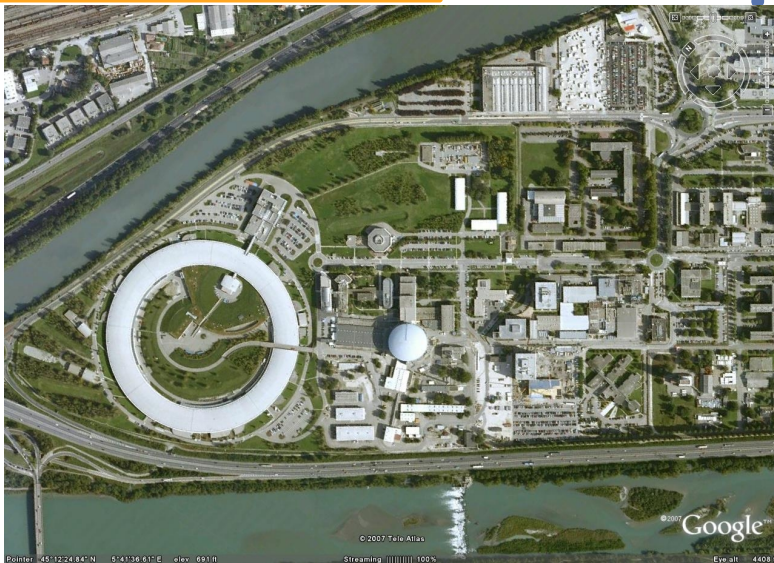
- Nano-Science and Nano-technology.
- Pump–Probe Experiments and Time–resolved Diffraction.
- Science at Extreme Conditions.
- Structural and Functional Biology and Soft Matter Science.
- X–ray Imaging.

Site Plan



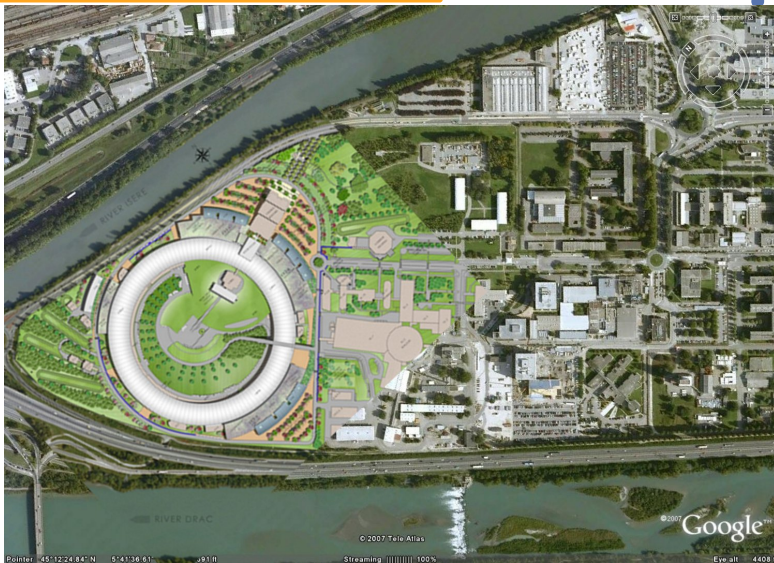
The ESRF Today

European Synchrotron Radiation Facility
A Light For Science

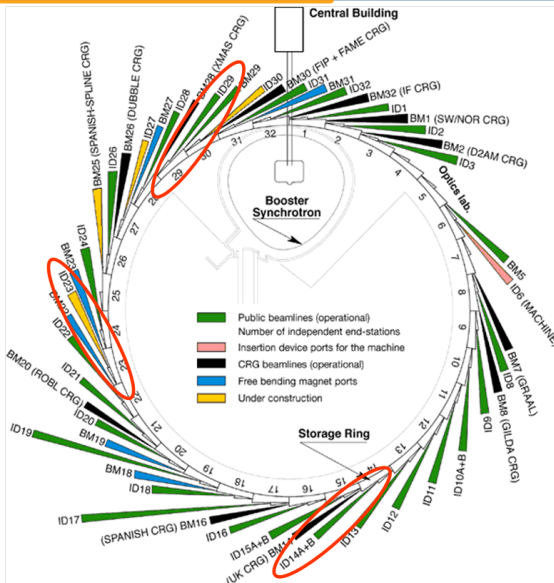


The ESRF Upgraded

European Synchrotron Radiation Facility
A Light For Science



Structural Biology at ESRF



Aim

- To provide across the suite of the **Structural Biology** beamlines a range of facilities spanning likely needs over next decade.

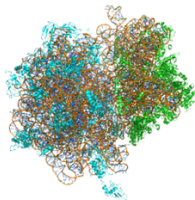
Increasing Complexity

1965

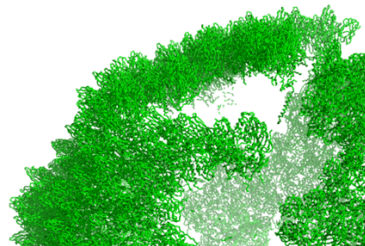
15 kDa



2.7 MDa



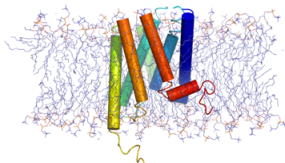
66 MDa



2004

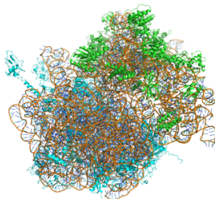
Kissing Frogs

GPCR



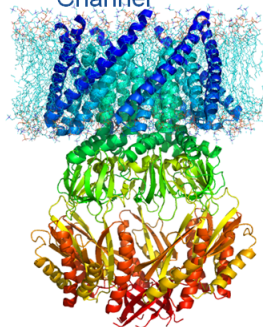
1043 crystals (3 positions)

Ribosome



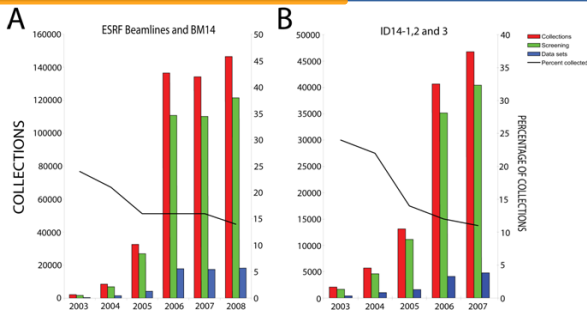
Thousands of thousands

Mechanoselective
Channel



“Many hundreds”

More Frogs



Observations from a Reliable Sample Changer.

Having a reasonably reliable sample changer helped acceptance of the organisational changes and investment required. Groups with well characterised samples collect from 1 in 4 crystals on average, some groups collect from 1 in 15 or fewer.

How is Beamtime Used?

- All samples are screened on all beamlines.
- Roughly one in 6 crystals are “okay”

For One Group.

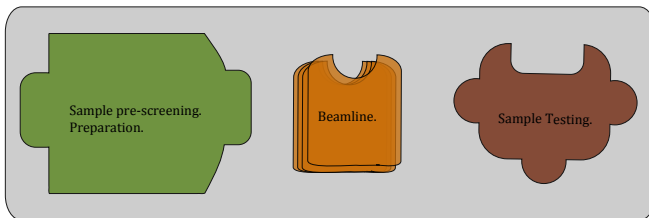
- **ID14-2** 0.02% of samples **tested** are collected on this beamline.
- **ID23-2** 8% of samples **tested** are collected on this beamline.

Conclusion

A dedicated screeningsample evaluation facility will provide more data collection time on the “optimised” beamlines.

Aims and concepts

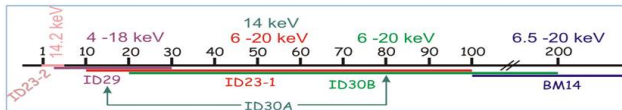
A plan has been generated along with our User community. This plan links all Structural Biology Group beamlines in co-operative upgrades. The expectation is to achieve more in this way than we would treating each individually. Multi-disciplinary research should be enabled.



Synopsis of Changes.

Beamline consequences

- ID14
 - rebuilt on ID30.
 - Canted: MAD ($20\mu m - 100\mu m$) and Evaluation.
- ID23
 - ID23-1 variable beamsizes 10-100 μm .
 - ID23-2 beam either 1. μm or 5 μm (Actually 3.5 by 7 μm^2)
- ID29
 - Convert for long wavelength experiments.
 - micro-beam MAD.



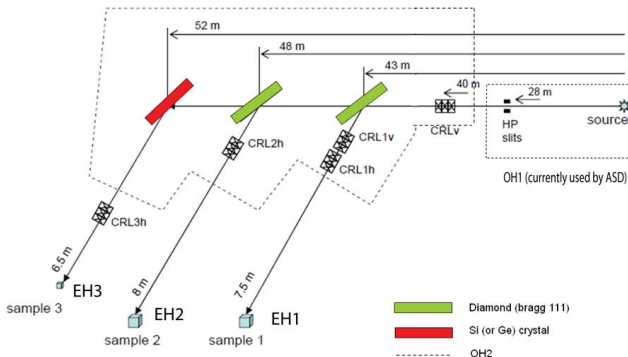
The Thinking Behind

The Process.

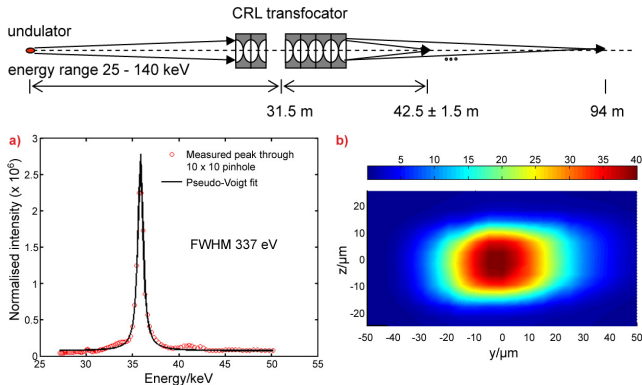
- Find the “BEST” crystal.
- Understand the diffraction properties of this crystal.
- Perform the best experiment.

However, the Diffraction experiment is a means to the end not the object in itself. Implementation must enable access to the Biological question.

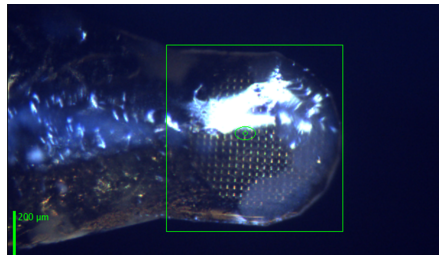
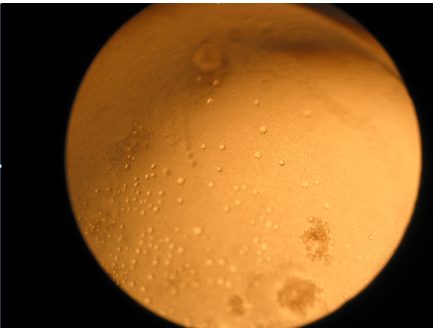
UPBL10 - MASSIF



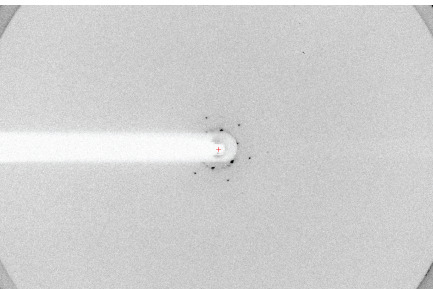
Implementation.



Micro-Beam Micro Xtal.

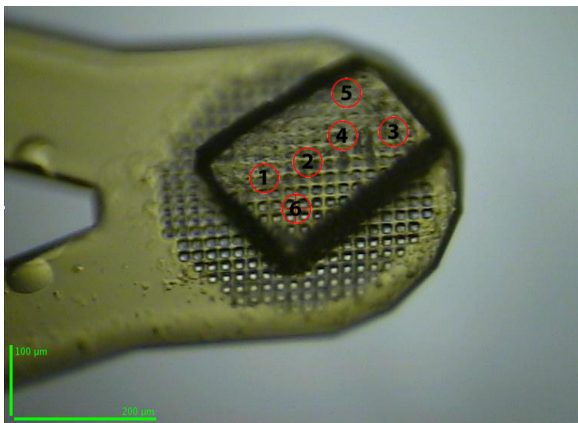


Micro-Beam Micro Xtal.

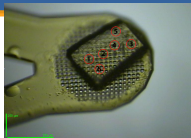


- Not all diffraction will be high resolution.
- Multi-disciplinary research to lead Scientific output.
- Feedback from diffraction to constructs, crystallisation, crystal handling.
- Scanning the loop completely would have required more than 2000 test shots.

Micro-Beam Big Xtal



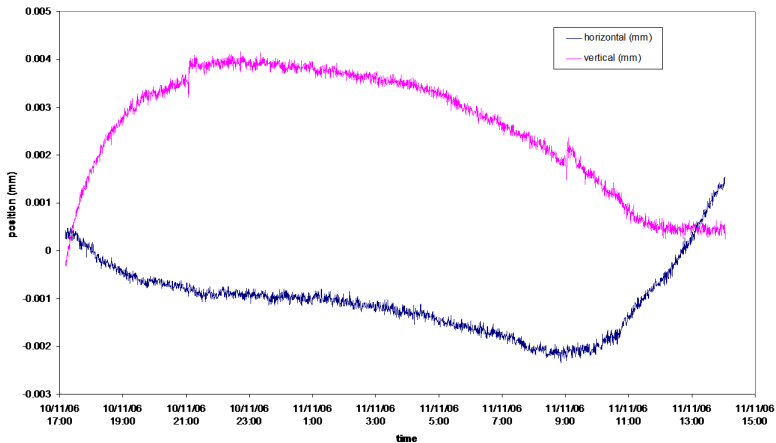
Micro-Beam Big Xtal



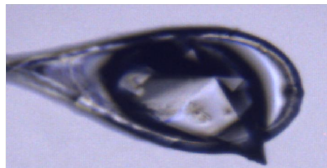
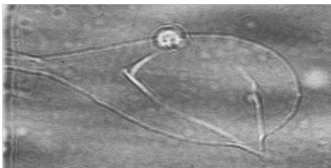
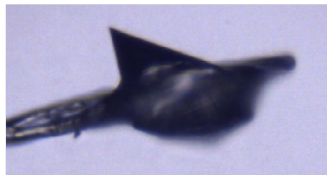
Posn	$d_{\min}(\text{\AA})$	$T_{\text{tot}}(\text{s})$	$\langle I/\sigma(I) \rangle$	$\Delta\phi_{T_{\text{tot}}}$	RHL	$\Delta\phi_{\text{tot}}$
1	1.8	40.0	9.2	70	0.09	390
2	4.0	114.6	9.2	105	0.81	65
3	1.7	69.0	9.0	69	0.05	690
4	2.1	69.0	7.8	69	0.25	138
5	1.8	75.0	9.1	75	.16	234
6	4.9	-	-	-	-	-

: Statistics from indexing and planning data collection from each of the points. T_{tot} = Time to reach $\langle I/\sigma(I) \rangle = 10$ at $d_{\min} = 4.0\text{\AA}$;
 RHL=Ratio Henderson Limit = [X-ray flux]/Time to HL;
 $\Delta\phi_{\text{tot}} = \Delta\phi_{T_{\text{tot}}} / (\text{RHL} \times 2)$

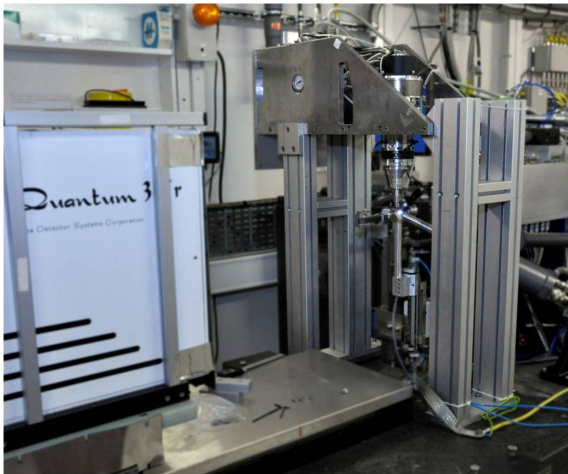
Stability



Finding Crystals

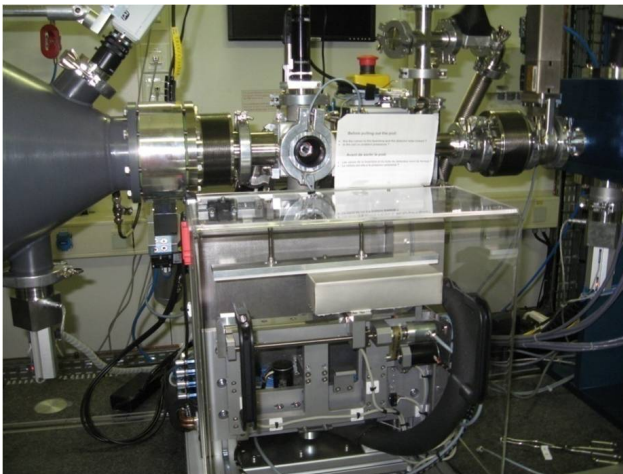


sub-micron spindle.



multi-disciplinary

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Challenges.

Software

- Optimise signal to noise from few, test images.
- Identify isomorphous classes of samples.
- Predict Radiation Damage and devise suitable strategy.
- Anomalous scattering and suitable strategies...
- Multiple crystals for data sets.
- Sample and information tracking...

Hardware.

- A simple, accurate, high density, robust sample holder.
- Robotics for rapid, automated sample characterisation and sorting.
- Provision of variable beam size over the operational range.
- Goniometer consistent with small beams and rapid automation.

PHASE 1

(i) Screening Station for frozen crystals mounted on Spine sample holders and for crystals in SBS crystallization plates.

(ii) High Speed Crystal Centring: New hardware and software for high speed crystal centring.

(iii) Native State Crystal Screening: Open the Native State crystals screening method to external users through the EMBL-PSB crystallization facility.

(iv) Equip 3 beamline stations with crystal screening/data collection stations

PHASE 2

(v) High Density Sample Holders for frozen crystals: Develop compact and intrinsically precise sample holder. Develop related storage and transport devices adapted to robotised handling

(vi) Screening/sorting environment for High Density Sample Holders: Develop tools for the screening station to screen samples in few tens of seconds, to sort the crystals in different pucks for data collection on different beamlines, and to manipulate automatically the pucks.

